

About the aromaticity of *symm*-triaminotrinitrobenzene.

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Streszczenie

Aromaticity and structural features of the isolated *symm*-triaminotrinitrobenzene (TATB) were examined using the nonempirical ab initio quantum chemical method and molecular dynamics at the Car-Parrinello level. Different criteria of the aromaticity were combined with the study of conformational flexibility of molecule and analysis of the electron density distribution. It was found that the cooperative effect of the resonance-assisted hydrogen bonds results in the ultimate decreasing aromaticity of the benzene ring in TATB. Values of the HOMA index indicate that it could be classified as low-aromatic in equilibrium state at zero temperature but completely nonaromatic at room temperature. An extremely high flexibility of the molecule is also not typical for aromatic rings. The electron delocalization in H-bonded O=N-C=C-N-H quasi-aromatic rings was found to be greater than that in the benzene ring of TATB.

Adres publiczny

<http://dx.doi.org/10.1021/acs.jpca.9b00433>

Strona internetowa wydawcy

<https://www.acs.org/content/acs/en.html>